

n,n-bis(2-cyanoethyl)aspartic acid
6328-90-1 | DTXSID20286167

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 38.3 L/kg

Global applicability domain: Inside

Local applicability domain index: 3.87e-01

Confidence level: 6.63e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Dicrotophos</div> <div>Measured: 45.7</div> <div>Predicted: 43.3</div>	<div>Image not found</div> <div>Metribuzin</div> <div>Measured: 51.3</div> <div>Predicted: 57.9</div>	<div>Image not found</div> <div>Uracil mustard</div> <div>Measured: 28.8</div> <div>Predicted: 37.5</div>
<div>Image not found</div> <div>Phosphamidon</div> <div>Measured: 7.08</div> <div>Predicted: 11.6</div>	<div>Image not found</div> <div>Metamitron</div> <div>Measured: 148</div> <div>Predicted: 126</div>	